Stephan Kupfer

List of Publications by Year
in descending order

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92 papers	1,794 citations	218381 26 h-index	329751 37 g-index
98 all docs	98 docs citations	98 times ranked	2070 citing authors

#	Article	IF	Citations
1	Intrinsic self-healing polymers with a high E-modulus based on dynamic reversible urea bonds. NPG Asia Materials, 2017, 9, e420-e420.	3.8	97
2	4-Methoxy-1,3-thiazole based donor-acceptor dyes: Characterization, X-ray structure, DFT calculations and test as sensitizers for DSSC. Dyes and Pigments, 2012, 94, 512-524.	2.0	67
3	Spatial resolution of tip-enhanced Raman spectroscopy â€“ DFT assessment of the chemical effect. Nanoscale, 2016, 8, 10229-10239.	2.8	64
4	Protonation effects on the resonance Raman properties of a novel (terpyridine)Ru(4H-imidazole) complex: an experimental and theoretical case study. Physical Chemistry Chemical Physics, 2011, 13, 15580.	1.3	54
5	Self-healing mechanism of metallopolymers investigated by QM/MM simulations and Raman spectroscopy. Physical Chemistry Chemical Physics, 2014, 16, 12422.	1.3	53
6	A SERS-based molecular sensor for selective detection and quantification of copper(II) ions. Sensors and Actuators B: Chemical, 2019, 279, 230-237.	4.0	51
7	Cu(<scp>i</scp>) vs. Ru(<scp>ii</scp>) photosensitizers: elucidation of electron transfer processes within a series of structurally related complexes containing an extended Ï€-system. Physical Chemistry Chemical Physics, 2018, 20, 24843-24857.	1.3	50
8	Dramatic Alteration of ³ILCT Lifetimes Using Ancillary Ligands in [Re(L)(CO)₃(phen-TPA)]ⁿ⁺ Complexes: An Integrated Spectroscopic and Theoretical Study. Journal of the American Chemical Society, 2018, 140, 4534-4542.	6.6	49
9	Resonance-Raman spectro-electrochemistry of intermediates in molecular artificial photosynthesis of bimetallic complexes. Chemical Communications, 2014, 50, 5227.	2.2	48
10	An artificial photosynthetic system for photoaccumulation of two electrons on a fused dipyridophenazine (dppz)â€“pyridoquinolinone ligand. Chemical Science, 2018, 9, 4152-4159.	3.7	48
11	[FeFe]-Hydrogenase H-cluster mimics mediated by naphthalene monoimide derivatives of peri-substituted dichalcogenides. Dalton Transactions, 2017, 46, 11180-11191.	1.6	43
12	Structural Control of Photoinduced Dynamics in 4H-Imidazole-Ruthenium Dyes. Journal of Physical Chemistry C, 2012, 116, 25664-25676.	1.5	38
13	An Assessment of RASSCF and TDDFT Energies and Gradients on an Organic Donorâ€“Acceptor Dye Assisted by Resonance Raman Spectroscopy. Journal of Chemical Theory and Computation, 2013, 9, 543-554.	2.3	38
14	Trapped in Imidazole: How to Accumulate Multiple Photoelectrons on a Blackâ€Absorbing Ruthenium Complex. Chemistry - A European Journal, 2014, 20, 3793-3799.	1.7	38
15	The Selfâ€Healing Potential of Triazoleâ€Pyridineâ€Based Metallopolymers. Macromolecular Rapid Communications, 2015, 36, 604-609.	2.0	37
16	Photochemistry and Electron Transfer Kinetics in a Photocatalyst Model Assessed by Marcus Theory and Quantum Dynamics. Journal of Physical Chemistry C, 2017, 121, 16066-16078.	1.5	35
17	Sterically induced distortions of nickel(II) porphyrins â€“ Comprehensive investigation by DFT calculations and resonance Raman spectroscopy. Coordination Chemistry Reviews, 2018, 360, 1-16.	9.5	35
18	Photophysics of Ru(II) Dyads Derived from Pyrenyl-Substitued Imidazo[4,5-f][1,10]phenanthroline Ligands. Journal of Physical Chemistry A, 2015, 119, 3986-3994.	1.1	34

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19	Unraveling the Lightâ€Activated Reaction Mechanism in a Catalytically Competent Key Intermediate of a Multifunctional Molecular Catalyst for Artificial Photosynthesis. Angewandte Chemie - International Edition, 2019, 58, 13140-13148.	7.2	34
20	Active repair of a dinuclear photocatalyst for visible-light-driven hydrogen production. Nature Chemistry, 2022, 14, 500-506.	6.6	32
21	A Novel Ru(II) Polypyridine Black Dye Investigated by Resonance Raman Spectroscopy and TDDFT Calculations. Journal of Physical Chemistry C, 2012, 116, 19968-19977.	1.5	30
22	Influence of Protonation State on the Excited State Dynamics of a Photobiologically Active Ru(II) Dyad. Journal of Physical Chemistry A, 2016, 120, 6379-6388.	1.1	29
23	The chemical effect goes resonant â€“ a full quantum mechanical approach on TERS. Nanoscale, 2020, 12, 6346-6359.	2.8	29
24	pysisyphus: Exploring potential energy surfaces in ground and excited states. International Journal of Quantum Chemistry, 2021, 121, e26390.	1.0	29
25	Influence of Multiple Protonation on the Initial Excitation in a Black Dye. Journal of Physical Chemistry C, 2011, 115, 24004-24012.	1.5	28
26	Arylamineâ€Modified Thiazoles as Donorâ€“Acceptor Dyes: Quantum Chemical Evaluation of the Chargeâ€Transfer Process and Testing as Ligands in Ruthenium(II) Complexes. European Journal of Organic Chemistry, 2012, 2012, 5231-5247.	1.2	26
27	Theoretical Assessment of Excited State Gradients and Resonance Raman Intensities for the Azobenzene Molecule. Journal of Chemical Theory and Computation, 2017, 13, 1263-1274.	2.3	26
28	Photophysics of BODIPY Dyes as Readily-Designable Photosensitisers in Light-Driven Proton Reduction. Inorganics, 2017, 5, 21.	1.2	25
29	Ultrafast Intramolecular Relaxation and Waveâ€Packet Motion in a Rutheniumâ€Based Supramolecular Photocatalyst. Chemistry - A European Journal, 2015, 21, 7668-7674.	1.7	24
30	Co-facial Ï€â€“Ï€ Interaction Expedites Sensitizer-to-Catalyst Electron Transfer for High-Performance CO₂ Photoreduction. Jacs Au, 2022, 2, 1359-1374.	3.6	24
31	Tuning of photocatalytic activity by creating a tridentate coordination sphere for palladium. Dalton Transactions, 2014, 43, 11676.	1.6	23
32	Light-responsive paper strips as CO-releasing material with a colourimetric response. Chemical Science, 2017, 8, 6555-6560.	3.7	23
33	A Ï€Ï€* State Enables Photoaccumulation of Charges on a Ï€-Extended Dipyridophenazine Ligand in a Ru(II) Polypyridine Complex. Journal of Physical Chemistry C, 2018, 122, 83-95.	1.5	19
34	Molecular Scylla and Charybdis: Maneuvering between pH Sensitivity and Excited-State Localization in Ruthenium Bi(benz)imidazole Complexes. Inorganic Chemistry, 2020, 59, 12097-12110.	1.9	19
35	Excited-State Switching in Rhenium(I) Bipyridyl Complexes with Donorâ€“Donor and Donorâ€“Acceptor Substituents. Journal of the American Chemical Society, 2021, 143, 9082-9093.	6.6	19
36	In situ spectroelectrochemical and theoretical study on the oxidation of a 4H-imidazole-ruthenium dye adsorbed on nanocrystalline TiO₂thin film electrodes. Physical Chemistry Chemical Physics, 2015, 17, 29637-29646.	1.3	16

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37	And yet they glow: thiazole based pushâ€“pull fluorophores containing nitro groups and the influence of regioisomerism. Methods and Applications in Fluorescence, 2015, 3, 025005.	1.1	16
38	Excited-State Switching Frustrates the Tuning of Properties in Triphenylamine-Donor-Ligand Rhenium(I) and Platinum(II) Complexes. Inorganic Chemistry, 2020, 59, 6736-6746.	1.9	16
39	Chemical Enhancement vs Moleculeâ€“Substrate Geometry in Plasmon-Enhanced Spectroscopy. ACS Photonics, 2021, 8, 2243-2255.	3.2	16
40	Hydrogen Production at a NiO Photocathode Based on a Ruthenium Dyeâ€“Cobalt Diimine Dioxime Catalyst Assembly: Insights from Advanced Spectroscopy and Post-operando Characterization. ACS Applied Materials & Interfaces, 2021, 13, 49802-49815.	4.0	16
41	Effect of the Catalytic Center on the Electron Transfer Dynamics in Hydrogen-Evolving Ruthenium-Based Photocatalysts Investigated by Theoretical Calculations. Journal of Physical Chemistry C, 2019, 123, 16003-16013.	1.5	15
42	Twoâ€Photonâ€Induced COâ€Releasing Molecules as Molecular Logic Systems in Solution, Polymers, and Cells. Chemistry - A European Journal, 2019, 25, 8453-8458.	1.7	15
43	Excitation Energy-Dependent Branching Dynamics Determines Photostability of Iron(II)â€“Mesoionic Carbene Complexes. Inorganic Chemistry, 2021, 60, 9157-9173.	1.9	15
44	Sensitization of NOâ€Releasing Ruthenium Complexes to Visible Light. Chemistry - A European Journal, 2015, 21, 15554-15563.	1.7	14
45	Photophysics of a Ruthenium 4Hâ€imidazole Panchromatic Dye in Interaction with Titanium Dioxide. ChemPhysChem, 2015, 16, 1061-1070.	1.0	14
46	Extended charge accumulation in rutheniumâ€“4H-imidazole-based black absorbers: a theoretical design concept. Physical Chemistry Chemical Physics, 2016, 18, 13357-13367.	1.3	13
47	Role of MLCT States in the Franckâ€“Condon Region of Neutral, Heteroleptic Cu(I)â€“4H-imidazolate Complexes: A Spectroscopic and Theoretical Study. Journal of Physical Chemistry A, 2020, 124, 6607-6616.	1.1	13
48	Covalent Linkage of BODIPYâ€Photosensitizers to Andersonâ€Type Polyoxometalates Using CLICK Chemistry. Chemistry - A European Journal, 2021, 27, 17181-17187.	1.7	13
49	Are charged tips driving TERS-resolution? A full quantum chemical approach. Journal of Chemical Physics, 2021, 154, 034106.	1.2	13
50	Synthesis, properties and quantum chemical evaluation of solvatochromic pyridinium-phenyl-1,3-thiazol-4-olate betaine dyes. Tetrahedron, 2013, 69, 1489-1498.	1.0	12
51	Theoretical Investigation of the Electronâ€Transfer Dynamics and Photodegradation Pathways in a Hydrogenâ€Evolving Rutheniumâ€“Palladium Photocatalyst. Chemistry - A European Journal, 2018, 24, 11166-11176.	1.7	12
52	Excited state properties of a series of molecular photocatalysts investigated by time dependent density functional theory. Physical Chemistry Chemical Physics, 2019, 21, 9052-9060.	1.3	12
53	Photo-Induced Charge Separation vs. Degradation of a BODIPY-Based Photosensitizer Assessed by TDDFT and RASPT2. Catalysts, 2018, 8, 520.	1.6	11
54	Metalâ€Free Aryl Crossâ€Coupling Directed by Traceless Linkers. Chemistry - A European Journal, 2019, 25, 16068-16073.	1.7	11

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55	Photochlorination of toluene â€“ the thin line between intensification and selectivity. Part 2: selectivity. Reaction Chemistry and Engineering, 2021, 6, 90-99.	1.9	11
56	Synthesis of three series of ruthenium tris-diimine complexes containing acridine-based Ï€-extended ligands using an efficient â€œchemistry on the complexâ€•approach. Dalton Transactions, 2016, 45, 16298-16308.	1.6	10
57	Photophysics of a Ruthenium Complex with a Ï€-Extended Dipyridophenazine Ligand for DNA Quadruplex Labeling. Journal of Physical Chemistry A, 2018, 122, 6558-6569.	1.1	10
58	Visible light-activated biocompatible photo-CORM for CO-release with colorimetric and fluorometric dual turn-on response. Polyhedron, 2019, 172, 175-181.	1.0	10
59	A Highly Fluorescent Dinuclear Aluminium Complex with Nearâ€Unity Quantum Yield**. Angewandte Chemie - International Edition, 2022, 61, .	7.2	10
60	Highly fluorescent single crystals of a 4-ethoxy-1,3-thiazole. Dyes and Pigments, 2018, 149, 644-651.	2.0	9
61	Unraveling the Lightâ€Activated Reaction Mechanism in a Catalytically Competent Key Intermediate of a Multifunctional Molecular Catalyst for Artificial Photosynthesis. Angewandte Chemie, 2019, 131, 13274-13282.	1.6	9
62	Resonance Raman Spectro-Electrochemistry to Illuminate Photo-Induced Molecular Reaction Pathways. Molecules, 2019, 24, 245.	1.7	9
63	Reaction Mechanism of Pdâ€Catalyzed â€œCOâ€Freeâ€•Carbonylation Reaction Uncovered by In Situ Spectroscopy: The Formyl Mechanism. Angewandte Chemie - International Edition, 2021, 60, 3422-3427.	7.2	9
64	Z-Selective phosphine promoted 1,4-reduction of ynoates and propynoic amides in the presence of water. Organic and Biomolecular Chemistry, 2021, 19, 6092-6097.	1.5	9
65	Deepâ€Red Luminescent Molybdenum(0) Complexes with Biâ€•and Tridentate Isocyanide Chelate Ligands. ChemPhotoChem, 2022, 6, .	1.5	9
66	Spectroelectrochemical Investigation of the Oneâ€Electron Reduction of Nonplanar Nickel(II) Porphyrins. ChemPhysChem, 2016, 17, 3480-3493.	1.0	8
67	Iron(0)â€Mediated Stereoselective (3+2)â€Cycloaddition of Thiochalcones via a Diradical Intermediate. Chemistry - A European Journal, 2020, 26, 11412-11416.	1.7	8
68	Hydrogel-Embedded Model Photocatalytic System Investigated by Raman and IR Spectroscopy Assisted by Density Functional Theory Calculations and Two-Dimensional Correlation Analysis. Journal of Physical Chemistry A, 2018, 122, 2677-2687.	1.1	7
69	Towards synthetic unimolecular [Fe2S2]-photocatalysts sensitized by perylene dyes. Dyes and Pigments, 2022, 198, 109940.	2.0	7
70	Novel [FeFe]-Hydrogenase Mimics: Unexpected Course of the Reaction of Ferrocenyl Î±-Thienyl Thioketone with Fe3(CO)12. Materials, 2022, 15, 2867.	1.3	7
71	Fate of Photoexcited Molecular Antennae - Intermolecular Energy Transfer versus Photodegradation Assessed by Quantum Dynamics. Journal of Physical Chemistry C, 2018, 122, 3273-3285.	1.5	6
72	A Molecular Photosensitizer in a Porous Block Copolymer Matrixâ€Implications for the Design of Photocatalytically Active Membranes. Chemistry - A European Journal, 2021, 27, 17049-17058.	1.7	6

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73	Activating a [FeFe] Hydrogenase Mimic for Hydrogen Evolution under Visible Light**. Angewandte Chemie - International Edition, 2022, , .	7.2	6
74	Unravelling the Mystery: Enlightenment of the Uncommon Electrochemistry of Naphthalene Monoimide [FeFe] Hydrogenase Mimics. European Journal of Inorganic Chemistry, 2022, 2022, .	1.0	6
75	Singlet oxygen generation versus Oâ€“O homolysis in phenyl-substituted anthracene endoperoxides investigated by RASPT2, CASPT2, CC2, and TD-DFT methods. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	5
76	Synthesis and Characterization of Ga^{III}, In^{III} and Lu^{III} Complexes of a Set of dtpa Bisâ€Amide Ligands. European Journal of Inorganic Chemistry, 2015, 2015, 4125-4137.	1.0	5
77	Modulating the Excited-State Decay Pathways of Cu(I) 4H-Imidazolate Complexes by Excitation Wavelength and Ligand Backbone. Journal of Physical Chemistry B, 2021, 125, 11498-11511.	1.2	5
78	Coupling of photoactive transition metal complexes to a functional polymer matrix**. Chemistry - A European Journal, 2021, 27, 17104-17114.	1.7	5
79	A Combined Spectroscopic and Theoretical Study on a Ruthenium Complex Featuring a Ï€â€Extended dppz Ligand for Lightâ€Driven Accumulation of Multiple Reducing Equivalents. Chemistry - A European Journal, 2022, 28, e202103882.	1.7	5
80	Ligandâ€Induced Donor State Destabilisation â€“ A New Route to Panchromatically Absorbing Cu(I) Complexes. Chemistry - A European Journal, 2022, , .	1.7	5
81	Lightâ€Driven Multiâ€Charge Separation in a Pushâ€Pull Rutheniumâ€Based Photosensitizer â€“ Assessed by RASSCF and TDDFT Simulations. ChemPhotoChem, 2022, 6, .	1.5	4
82	Tetraaryl Cyclopentadienones: Experimental and Theoretical Insights into Negative Solvatochromism and Electrochemistry. European Journal of Organic Chemistry, 2020, 2020, 6555-6562.	1.2	3
83	The role of anchoring groups in ruthenium(II)-bipyridine sensitized p-type semiconductor solar cellsâ€”a quantum chemical approach. Journal of Physics B: Atomic, Molecular and Optical Physics, 2020, 53, 234001.	0.6	3
84	Unusually Short-Lived Solvent-Dependent Excited State in a Half-Sandwich Ru(II) Complex Induced by Low-Lying ³MC States. Journal of Physical Chemistry A, 2018, 122, 1550-1559.	1.1	2
85	Tuning the metalâ€“ligand bond in theÏƒâ€complexes of stannylenes and azabenzenes. Journal of Computational Chemistry, 2021, 42, 2103-2115.	1.5	2
86	New insights into the biphasic â€œCO-freeâ€•Pausonâ€“Khand cyclisation reaction through combinedin situspectroscopy and multiple linear regression modelling. Catalysis Science and Technology, 2021, 11, 1626-1636.	2.1	1
87	Metalâ€“ligand bonding in tricarbonyliron(0) complexes bearing thiochalcone ligands. New Journal of Chemistry, 2022, 46, 12924-12933.	1.4	1
88	Frontispiece: Twoâ€Photonâ€Induced COâ€Releasing Molecules as Molecular Logic Systems in Solution, Polymers, and Cells. Chemistry - A European Journal, 2019, 25, .	1.7	0
89	A Highly Fluorescent Dinuclear Aluminium Complex with Nearâ€Unity Quantum Yield. Angewandte Chemie, 0, , .	1.6	0
90	Aktivierung eines biomimetischen [FeFe]â€Hydrogenaseâ€Komplexes fÃ¼r die H ₂ â€Produktion mit sichtbarem Licht**. Angewandte Chemie, 0, , .	1.6	0

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91	Frontispiz: Aktivierung eines biomimetischen [FeFe]â€Hydrogenaseâ€Komplexes fÃ¼r die H₂â€Produktion mit sichtbarem Licht. Angewandte Chemie, 2022, 134, .	1.6	0
92	Frontispiece: Activating a [FeFe] Hydrogenase Mimic for Hydrogen Evolution under Visible Light. Angewandte Chemie - International Edition, 2022, 61, .	7.2	0